

Reply to "Comment on 'Thomson rings in a disk' "

A. Puente

*Departament de Física, Universitat de les Illes Balears,
E-07122 Palma de Mallorca, Spain*

R.G. Nazmitdinov

*Departament de Física, Universitat de les Illes Balears,
E-07122 Palma de Mallorca, Spain and
Bogoliubov Laboratory of Theoretical Physics,
Joint Institute for Nuclear Research, 141980 Dubna, Russia*

M. Cerkaski

*Department of Theory of Structure of Matter,
Institute of Nuclear Physics PAN, 31-342 Cracow, Poland*

K.N. Pichugin

Kirensky Institute of Physics, 660036 Krasnoyarsk, Russia

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Abstract

We demonstrate that our model [Phys.Rev. E**91**, 032312 (2015)] serves as a useful tool to trace the evolution of equilibrium configurations of one-component charged particles confined in a disk. Our approach reduces significantly the computational effort in minimizing the energy of equilibrium configurations and demonstrates a remarkable agreement with the values provided by molecular dynamics calculations. We show that the comment misrepresents our paper, and fails to provide plausible arguments against the formation hexagonal structure for $n \geq 200$ in molecular dynamics calculations.

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In our recent publication [1], we have developed a semi-analytical approach that allows to determine equilibrium configurations for arbitrary, but finite, number of charged particles confined in a disk geometry. In the Comment [2] by Amore it was found that the minimum energy configuration of $N = 395$ charges confined in disk and interacting via the Coulomb potential has a lower energy than the result of our molecular dynamics (MD) calculations [1]. Based only on this result Amore concluded that *"...the formation of a hexagonal core and valence circular rings for the centered configurations, predicted by the model of Ref.[1], is not supported by numerical evidence and the configurations obtained with this model cannot be used as a guide for the numerical calculations, as claimed by the authors. In light of this findings, the validity of the model of Ref.[1] must be questioned, particular for $N \gtrsim 200$."*

Hereafter, for the sake of convenience we refer to our model as the circular model (CM). We agree with the author that his possible global MD minimum is better than our estimate for the particular case $N = 395$. However, this is not enough to conclude that the CM can not help to reduce substantially the computational effort in MD or simulated annealing (SA) calculations for the following reasons.

1. From the Monte Carlo and MD calculations, even for a relatively small number of charged particles, it follows that the amount of stable configurations grows very rapidly with the number of particles. Sometimes, metastable states with lower (or higher) symmetry are found with much higher probability than the true ground state. This fact was confirmed by the author who *"generated 3001 configurations ..."* to get just one instance of the improved $E_{\text{MIN}} = 110664.44$ new tentative ground state, with our prediction for the particle number at the boundary ring: *"... $N_p = 147$ charges are disposed on the border of the disk, in agreement with Ref.1"*. Evidently, in contrast to his claim, Amore has confirmed the usefulness of the CM.

Indeed, the particle number on the boundary ring N_p is one of the key elements for any calculation, since once it is defined, it is necessary to simulate less various configurations (with a number of charges $N - N_p$). We recall that $N_p \gg N_{p-1} > N_{p-2} > \dots > 1$, where p is a number of rings, and N is a total number of charges.

In fact, external ring occupations are extremely well predicted with some occasional ± 1 mismatch by means of the expression $N_p(N) = [2.795N^{2/3} - 3.184]$, where $p \simeq [\sqrt{N}/2]$ [1]. It is noteworthy that these expressions are obtained from the systematic CM

results.

2. In our publication [1], in order to obtain our estimate of the MD ground state E_{MD} , we generated only 100 configurations with the boundary ring $N_{p=9} = 147$ charges, where the internal charges were randomly distributed. As a result, we have obtained $E_{\text{CM}} = 110667.6 > E_{\text{MD}} = 110665.1 > E_{\text{MIN}} = 110664.44$. Note, however, that the disagreement between the author's new result and our model prediction E_{CM} is still less than $3 \times 10^{-3}\%$ (as we stated in our paper it is $2 \times 10^{-3}\%$). Moreover, the occupations for the external (approximately circular) shells are quite accurately predicted within CM for any N . In the case of $N = 395$ we have obtained $(147, 65, 50, 40)$, while the analysis of the Amore's MD ground state yields $(147, 66, 51, 40)$. This comparison suggests that the effectivity of the CM prediction might be improved if the second ring, the nearest neighbor to the boundary one, should be taken into account.
3. To prove the usefulness of this idea we consider initial configurations characterized by external occupations: $N_9 = 147$ (Set 1); $N_9 = 147$, $N_8 = 65$ (Set 2); $N_9 = 147$, $N_8 = 66$ (Set 3). In all cases we have generated 2000 configurations, where N_9 particles were initially set on the boundary at $R_1 = 1$, and for two other sets N_8 particles have been distributed at $R_2 = 0.96$. That value was chosen to take into account monopole oscillations around the equilibrium configuration. The remaining particles were distributed randomly.

For the Set 1 (Fig.1, top panel) we found the lowest state $E_{\text{MD}} = 110664.52 > E_{\text{MIN}} = 110664.44$, that occurs just once. In the middle panel (Set 2) we use two boundary shells $N_9 = 147$, $N_8 = 65$, predicted by the CM partition, and obtain slightly lower state. However, the ground state is not reached yet.

The systematic analysis of the CM results leads us to conclusion that the second shell occupation is fitted by the formula $N_{p-1}(N) = [1.351N^{2/3} - 6.566]$ that yields $N_8 = 66$. Considering the initial configuration with $N_9 = 147$, $N_8 = 66$ (Set 3) with randomly distributed internal charges (Fig.1, bottom panel), we obtain that the ground state E_{MIN} occurs three times (0.15%). In other words, with this initialization it appears once every 666 generated configurations. Note that Amore has generated 3001 configurations to obtain just one realization of the possible ground state.

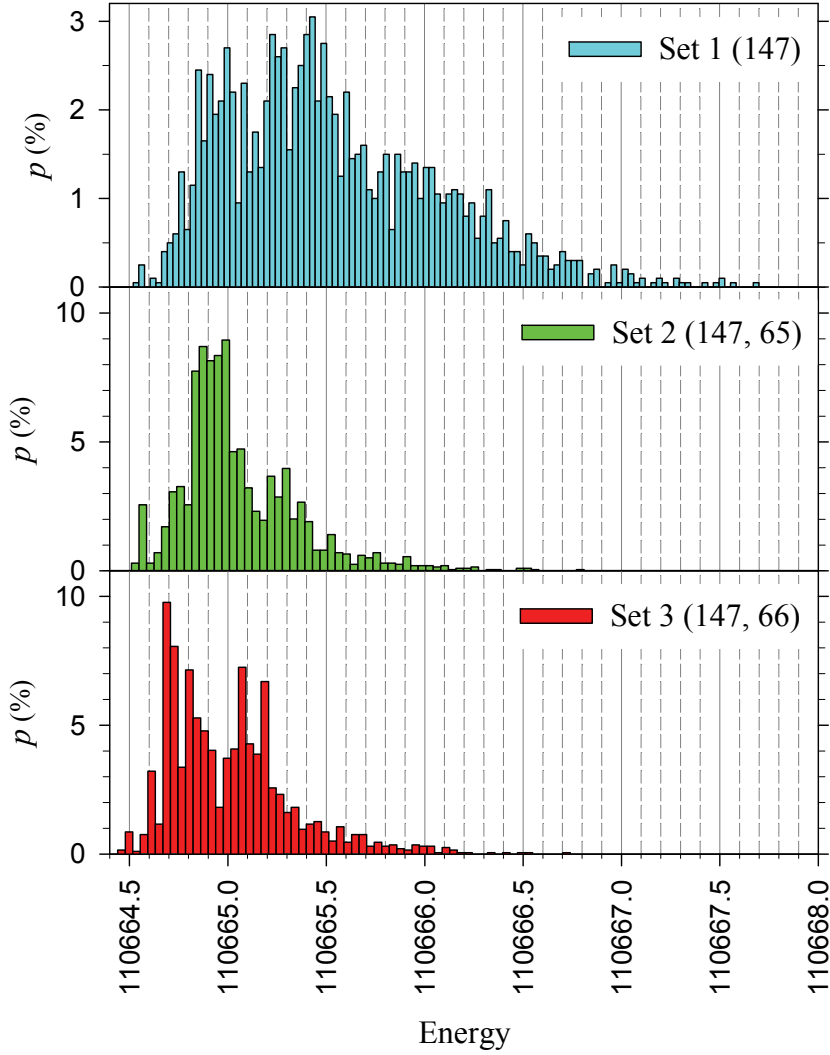


FIG. 1: (Color online) Histograms for energy states of $N = 395$ charges in the disk geometry obtained by means of the MD method for different initialization procedures.

4. We recall that for infinite systems the hexagonal lattice has the lowest energy of all two-dimensional Wigner Bravais crystals [3]. Evidently, the decrease of system size places primary emphasis upon system boundaries (see, for example, discussion in Refs.[4, 5]). Therefore, one needs to understand how the Wigner crystallization may settle down, in a particular, in a disk geometry as a function of the number of interacting charged particles. In Supplemental Material we compare our results

corresponding to the MD and the semi-analytical approach for $161 \leq N \leq 260$ charges. These results demonstrate a remarkable agreement between two approaches and make it clear how the centered hexagonal lattice (CHL) evolves with the increase of charge particle number. Therefore, we strongly believe that the results obtained by means of our method can be successfully used to feed SA or MD calculations with sensible initial configurations, reducing significantly the amount of scanning, normally needed to visit the global energy minima.

5. The systematic manifestation of the CHL with the increase of particle number $N \geq 200$ in our CM and MD results can be interpreted as the onset of the hexagonal crystallization in the disk geometry. There is no, however, any manifestation of a phase transition, typical for infinite systems. In a finite system a crossover takes place from the CHL to ring localization with the approaching to the disk boundary. This ring organization is clearly seen at the boundary in Fig.2 presented by the author (two clear rings).

In our paper we have compared the MD configuration with the prediction of the CM for the CHL at $N = 395$. In fact, in our MD calculations the clean CHL takes place at $N = 381$ with the configuration **143, 64, 49, 39, 30, 19, 18, 12, 6, 1** and the minimal energy $E = 102764.53$. The valence configurations with $N_7 = 49$, $N_8 = 64$, $N_9 = 143$ form well defined ring structure.

The increase of particle number disintegrates slowly the CHL in the disk geometry, while the hexagonal lattice still exists. Nevertheless, with each new shell, as soon as a new particle appears at the centre it gives rise to the CHL again. Since we deal with a finite system, restricted by the circular geometry, the boundary affects the plain symmetrical configurations giving rise to defects.

In conclusion, we disagree with the main outcome of the author's Comment formulated in his Summary. In order to argue against our model and corresponding conclusions, it is required a systematic thorough analysis of the system with increasing particle number but not only one particular case. In fact, we have demonstrated that the CM predictions for external rings (N_p, N_{p-1}) enable to us to reduce substantially scanning efforts needed to reach the ground state in the MD.

Acknowledgments

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- [1] M. Cerkaski, R.G. Nazmitdinov, and A.Puente, Phys. Rev. E**91**, 032312 (2015).
- [2] P. Amore, arXiv:1607.08785.
- [3] L. Bonsall and A.A. Maradudin, Phys. Rev. B**15**, 1959 (1977).
- [4] H. Saarikoski, S.M. Reimann, A. Harju, and M. Manninen, Rev. Mod. Phys. **82**, 2785 (2010).
- [5] J.L. Birman, R.G. Nazmitdinov, and V.I. Yukalov, Phys. Rep. **526**, 1 (2013).

Supplemental Material

The MD and Circular Model results

These tables summarize our results corresponding to the minimum energy equilibrium configurations under disk confinement. E_{MD} , E_{CM} are the total MD (our best estimate) and the Circular Model energies.

Results for $161 \leq n \leq 180$

n	E_{MD}	Configuration	E_{CM}	Configuration
161	17323.885	[79,33,22,15,9,3]	17324.571	[79,33,22,15,9,3]
162	17548.672	[79,33,23,15,9,3]	17549.325	[79,33,23,15,9,3]
163	17775.066	[80,33,23,15,9,3]	17775.717	[80,33,23,15,9,3]
164	18002.880	[80,33,23,16,9,3]	18003.488	[80,33,23,16,9,3]
165	18232.249	[80,34,23,16,9,3]	18232.837	[80,34,23,16,9,3]
166	18463.081	[81,34,23,16,9,3]	18463.668	[81,34,23,16,9,3]
167	18695.335	[81,34,24,16,9,3]	18695.901	[81,34,24,16,9,3]
168	18929.198	[81,34,24,16,10,3]	18929.751	[81,34,24,16,10,3]
169	19164.419	[81,34,24,16,10,4]	19164.969	[81,34,24,16,10,4]
170	19400.980	[82,34,24,16,10,4]	19401.528	[82,34,24,16,10,4]
171	19639.241	[82,35,24,16,10,4]	19639.768	[82,35,24,16,10,4]
172	19878.944	[83,35,24,16,10,4]	19879.461	[83,34,24,17,10,4]
173	20120.029	[83,35,24,17,10,4]	20120.507	[83,35,24,17,10,4]
174	20362.731	[83,35,25,17,10,4]	20363.180	[83,35,25,17,10,4]
175	20606.871	[84,35,25,17,10,4]	20607.318	[84,35,25,17,10,4]
176	20852.540	[84,35,25,17,11,4]	20852.999	[84,36,25,17,10,4]
177	21099.703	[84,36,25,17,11,4]	21100.164	[84,36,25,17,11,4]
178	21348.301	[85,36,25,17,11,4]	21348.762	[85,36,25,17,11,4]
179	21598.311	[85,36,25,18,11,4]	21598.791	[85,36,25,17,11,5]
180	21849.924	[85,36,25,18,11,5]	21850.334	[85,36,25,18,11,5]

Results for $181 \leq n \leq 207$

n	E_{MD}	Configuration	E_{CM}	Configuration
181	22102.961	[86,36,25,18,11,5]	22103.368	[86,36,25,18,11,5]
182	22357.440	[86,36,26,18,11,5]	22357.815	[86,36,26,18,11,5]
183	22613.517	[86,37,26,18,11,5]	22613.878	[86,37,26,18,11,5]
184	22871.031	[87,37,26,18,11,5]	22871.391	[87,37,26,18,11,5]
185	23129.918	[87,36,26,18,11,6,1]	23130.442	[87,37,26,18,12,5]
186	23390.285	[87,37,26,18,11,6,1]	23391.044	[87,37,26,19,12,5]
187	23652.188	[87,37,26,18,12,6,1]	23652.947	[87,37,26,18,12,6,1]
188	23915.459	[88,37,26,18,12,6,1]	23916.215	[88,37,26,18,12,6,1]
189	24180.381	[88,37,27,18,12,6,1]	24181.062	[88,37,26,19,12,6,1]
190	24446.798	[89,37,27,18,12,6,1]	24447.458	[88,37,27,19,12,6,1]
191	24714.561	[89,37,27,19,12,6,1]	24715.189	[89,37,27,19,12,6,1]
192	24983.853	[89,38,27,19,12,6,1]	24984.461	[89,38,27,19,12,6,1]
193	25254.755	[90,38,27,19,12,6,1]	25255.362	[90,38,27,19,12,6,1]
194	25527.119	[90,38,27,19,13,6,1]	25527.697	[90,38,27,19,13,6,1]
195	25801.014	[90,38,27,20,13,6,1]	25801.595	[90,38,28,19,13,6,1]
196	26076.378	[91,38,27,20,13,6,1]	26076.964	[91,38,28,19,13,6,1]
197	26353.122	[91,39,27,20,13,6,1]	26353.672	[91,38,27,20,13,7,1]
198	26631.365	[91,39,28,20,13,6,1]	26631.870	[91,39,27,20,13,7,1]
199	26911.103	[91,39,28,20,13,7,1]	26911.559	[91,39,28,20,13,7,1]
200	27192.287	[92,39,28,20,13,7,1]	27192.741	[92,39,28,20,13,7,1]
201	27475.149	[92,40,28,20,13,7,1]	27475.591	[92,40,28,20,13,7,1]
202	27759.495	[92,39,28,21,14,7,1]	27759.953	[93,40,28,20,13,7,1]
203	28045.151	[93,39,28,21,14,7,1]	28045.669	[93,40,29,20,13,7,1]
204	28332.320	[93,40,28,21,14,7,1]	28332.900	[93,40,29,20,14,7,1]
205	28621.069	[93,40,29,21,14,7,1]	28621.647	[93,40,29,21,14,7,1]
206	28911.236	[94,40,29,21,14,7,1]	28911.813	[94,40,29,21,14,7,1]
207	29203.054	[94,41,29,21,14,7,1]	29203.620	[94,41,29,21,14,7,1]

Results for $208 \leq n \leq 234$

n	E_{MD}	Configuration	E_{CM}	Configuration
208	29496.341	[94,40,29,21,14,8,2]	29496.944	[94,41,29,21,14,8,1]
209	29790.985	[95,40,29,21,14,8,2]	29791.618	[95,41,29,21,14,8,1]
210	30087.107	[95,41,29,21,14,8,2]	30087.834	[95,41,30,21,14,8,1]
211	30384.840	[95,41,30,21,14,8,2]	30385.659	[95,41,30,22,14,8,1]
212	30684.005	[96,41,30,21,14,8,2]	30684.828	[96,41,30,22,14,8,1]
213	30984.546	[96,41,30,22,14,8,2]	30985.505	[96,41,30,22,15,8,1]
214	31286.636	[96,41,30,22,13,9,3]	31287.674	[96,41,30,22,15,8,2]
215	31590.285	[97,41,30,22,13,9,3]	31591.327	[97,41,30,22,15,8,2]
216	31895.274	[97,41,30,22,14,9,3]	31896.396	[97,42,30,22,15,8,2]
217	32201.810	[97,41,30,22,15,9,3]	32202.828	[97,41,30,22,15,9,3]
218	32509.860	[97,42,30,22,15,9,3]	32510.843	[97,42,30,22,15,9,3]
219	32819.357	[98,42,30,22,15,9,3]	32820.338	[98,42,30,22,15,9,3]
220	33130.391	[98,42,31,22,15,9,3]	33131.367	[98,42,31,22,15,9,3]
221	33443.063	[98,42,31,23,15,9,3]	33444.031	[98,42,31,23,15,9,3]
222	33757.067	[99,42,31,23,15,9,3]	33758.034	[99,42,31,23,15,9,3]
223	34072.594	[99,42,31,23,16,9,3]	34073.531	[99,42,31,23,16,9,3]
224	34389.617	[99,43,31,23,16,9,3]	34390.523	[99,43,31,23,16,9,3]
225	34708.151	[100,43,31,23,16,9,3]	34709.055	[100,43,31,23,16,9,3]
226	35028.160	[100,43,31,23,15,10,4]	35029.106	[100,43,31,23,16,9,4]
227	35349.639	[100,43,31,23,16,10,4]	35350.486	[100,43,31,23,16,10,4]
228	35672.675	[101,43,31,23,16,10,4]	35673.518	[101,43,31,23,16,10,4]
229	35997.082	[101,43,32,23,16,10,4]	35997.893	[101,43,32,23,16,10,4]
230	36323.076	[101,44,32,23,16,10,4]	36323.861	[101,44,32,23,16,10,4]
231	36650.589	[101,44,32,24,16,10,4]	36651.395	[101,44,32,24,16,10,4]
232	36979.503	[102,44,32,24,16,10,4]	36980.306	[102,44,32,24,16,10,4]
233	37309.955	[102,44,32,24,17,10,4]	37310.715	[102,44,32,24,17,10,4]
234	37642.049	[102,44,33,24,17,10,4]	37642.792	[102,44,33,24,17,10,4]

Results for $235 \leq n \leq 260$

n	E_{MD}	Configuration	E_{CM}	Configuration
235	37975.484	[103,44,33,24,17,10,4]	37976.225	[103,44,33,24,17,10,4]
236	38310.462	[103,44,33,24,17,11,4]	38311.186	[103,45,33,24,17,10,4]
237	38646.933	[103,45,33,24,17,11,4]	38647.705	[103,45,33,24,17,11,4]
238	38984.913	[104,45,33,24,17,11,4]	38985.683	[104,45,33,24,17,11,4]
239	39324.318	[104,45,33,25,16,11,5]	39325.033	[104,45,33,24,17,11,5]
240	39665.177	[104,45,33,25,14,12,6,1]	39665.976	[104,45,33,25,17,11,5]
241	40007.632	[104,45,33,25,15,12,6,1]	40008.473	[105,45,33,25,17,11,5]
242	40351.460	[105,45,33,25,15,12,6,1]	40352.337	[105,45,33,25,18,11,5]
243	40696.877	[105,45,33,25,16,12,6,1]	40697.757	[105,46,33,25,18,11,5]
244	41043.791	[105,46,33,25,16,12,6,1]	41044.696	[105,46,34,25,18,11,5]
245	41392.174	[106,46,33,25,16,12,6,1]	41393.091	[106,46,34,25,18,11,5]
246	41741.996	[106,46,34,25,16,12,6,1]	41743.132	[106,46,34,25,18,12,5]
247	42093.362	[106,46,34,25,17,12,6,1]	42094.661	[106,46,34,25,18,11,6,1]
248	42446.278	[107,46,34,25,17,12,6,1]	42447.440	[106,46,34,25,18,12,6,1]
249	42800.557	[107,46,34,25,18,12,6,1]	42801.689	[107,46,34,25,18,12,6,1]
250	43156.448	[107,46,34,26,18,12,6,1]	43157.543	[107,46,34,26,18,12,6,1]
251	43513.864	[107,47,34,26,18,12,6,1]	43514.922	[107,47,34,26,18,12,6,1]
252	43872.683	[108,47,34,26,18,12,6,1]	43873.737	[108,47,34,26,18,12,6,1]
253	44233.025	[108,47,35,26,18,12,6,1]	44234.016	[108,47,34,26,19,12,6,1]
254	44594.889	[108,47,35,26,19,12,6,1]	44595.833	[108,47,35,26,19,12,6,1]
255	44958.250	[109,47,35,26,19,12,6,1]	44959.191	[109,47,35,26,19,12,6,1]
256	45323.172	[109,47,35,26,19,13,6,1]	45324.102	[109,48,35,26,19,12,6,1]
257	45689.578	[109,48,35,26,19,13,6,1]	45690.514	[109,48,35,26,19,13,6,1]
258	46057.509	[110,48,35,26,19,13,6,1]	46058.440	[110,48,35,26,19,13,6,1]
259	46426.854	[110,48,35,27,19,13,6,1]	46427.711	[110,48,35,26,19,13,7,1]
260	46797.668	[110,48,35,27,19,13,7,1]	46798.489	[110,48,35,27,19,13,7,1]